Spectral Graph Theory
An Invitation

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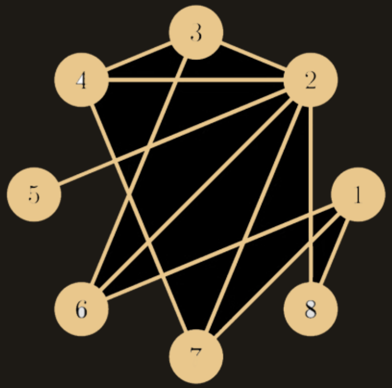
Eigenvalues of a Graph?



$$\vec{v} = \lambda \vec{v}$$

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OUTLINE

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BASIC GRAPH THEORY

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GRAPH LAPLACIAN AND ITS BASIC PROPERTIES

03
FIEDLER VECTOR AND FIEDLER VALUE OF A GRAPH

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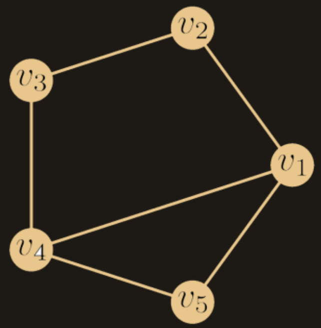
SPECTRAL EMBEDDING & CLUSTERING

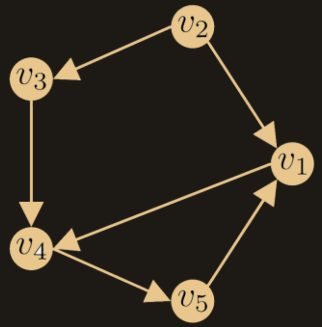
Basic Graph Theory



$$G = (V, E)$$

$$V = \{v_1, v_2, v_3, v_4, v_5\}$$

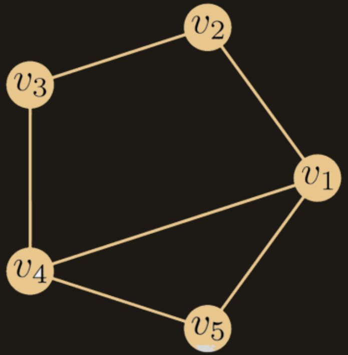
$$E = \{(v_1, v_2), (v_1, v_4), (v_2, v_3), \cdots, (v_5, v_1)\}$$



$$e_{1,2} = (v_1, v_2)$$

$$e_{2,1} = (v_2, v_1) \neq e_{1,2}$$

Degrees of Vertices and Connectivity



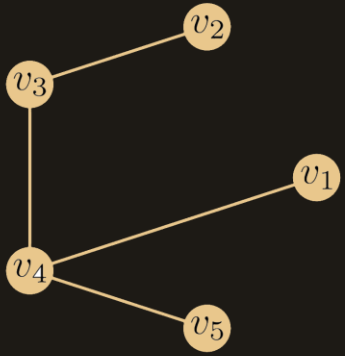
$d(v_1) = 3$

$d(v_2) = 2$

$d(v_3) = 2$

$d(v_4) = 3$

$d(v_5) = 2$



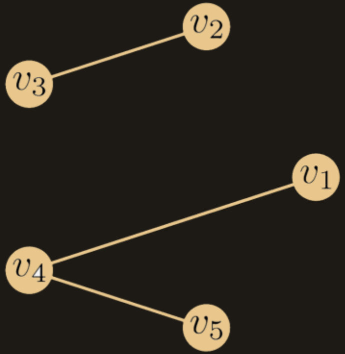
$d(v_1) = 1$

$d(v_2) = 1$

$d(v_3) = 2$

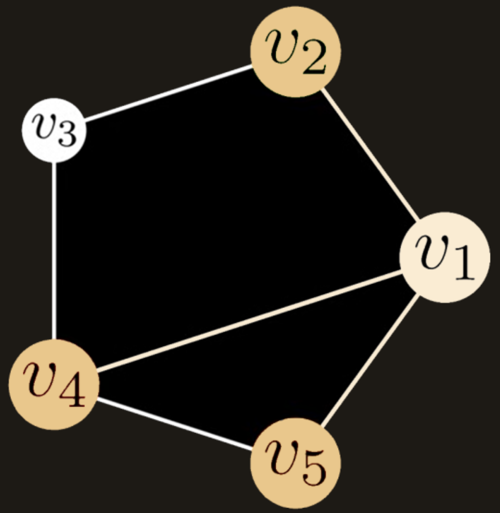
$d(v_4) = 3$

$d(v_5) = 1$



The graph has 2 connected components, but the graph itself is no longer connected.

Adjacency and Degree Matrices



$$\begin{pmatrix} 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \end{pmatrix}$$

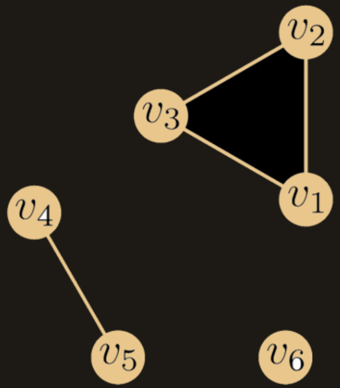
$$A_{i,j} = \begin{cases} 1 & \text{if } (v_i, v_j) \in E \\ 0 & \text{otherwise} \end{cases}$$

$$\begin{pmatrix} 3 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 0 & 2 \end{pmatrix}$$

$$D_{i,j} = \begin{cases} d(v_i) & \text{if } i = j \\ 0 & \text{otherwise} \end{cases}$$

- **Both matrices are real symmetric**

Disconnected graphs have distinct block structure of adjacency matrix



$$A: \begin{pmatrix} 0 & 1 & 1 & 0 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

- **This has interesting impact on eigenvalues and eigenvectors**

Spectral Theory of Graphs

In mathematics, spectral theory is an inclusive term for theories extending the eigenvector and eigenvalue theory of a single square matrix to a much broader theory of the structure of operators in a variety of mathematical spaces.

Source: Wikipedia

Real symmetric matrices are guaranteed to be diagonalizable with real eigenvalues

$$\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix} = \underbrace{\begin{pmatrix} -0.44 & -0.71 & 0.56 & 0.0 \\ -0.56 & 0.0 & -0.44 & -0.71 \\ -0.56 & 0.0 & -0.44 & 0.71 \\ -0.44 & 0.71 & 0.56 & 0.0 \end{pmatrix}}_{P} \underbrace{\begin{pmatrix} 2.6 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & -1.6 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}}_{\Lambda} \underbrace{\begin{pmatrix} -0.44 & -0.71 & 0.56 & 0.0 \\ -0.56 & 0.0 & -0.44 & -0.71 \\ -0.56 & 0.0 & -0.44 & 0.71 \\ -0.44 & 0.71 & 0.56 & 0.0 \end{pmatrix}^{-1}}_{P^{-1}}$$

Addition and subtraction retain real symmetric property

$$\underbrace{\begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 2 \end{pmatrix}}_{D} - \underbrace{\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{pmatrix}}_{A} = \underbrace{\begin{pmatrix} 2 & -1 & -1 & 0 \\ -1 & 3 & -1 & -1 \\ -1 & -1 & 3 & -1 \\ 0 & -1 & -1 & 2 \end{pmatrix}}_{\text{Laplacian matrix: } \boldsymbol{L}}$$

$$L_{ij} = \begin{cases} d(v_i) & \text{if } i = j \\ -1 & \text{if } i \neq j \text{ and } v_i \text{ is adjacent to } v_j \\ 0 & \text{otherwise} \end{cases}$$

Graph Laplacian

$$L = D - A$$

$$(Lf)_i = \sum_{j, i \sim j} (f(i) - f(j))$$

$$Lf = \lambda f$$

$$\lambda = f^t L f$$

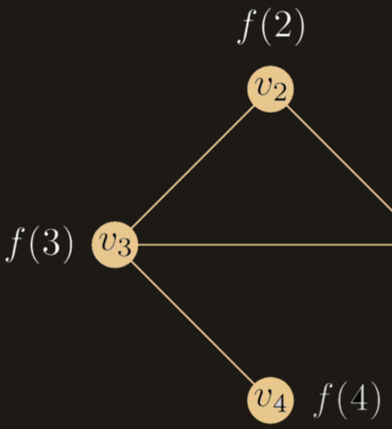
$$\lambda = f^t L f = \sum_i f(i) (Lf)_i$$

$$\lambda = \sum_i (f(i) \sum_{j, i \sim j} (f(i) - f(j)))$$

- f is a function on graph vertices and an eigenvector of Laplacian

Graph Laplacian

$$\lambda = \sum_i \left(f(i) \sum_{j, i\sim j} (f(i) - f(j))\right)$$



$$\begin{gathered} f(1)(f(1) - f(2)) + f(1)(f(1) - f(3)) \\ + \\ f(2)(f(2) - f(1)) + f(2)(f(2) - f(3)) \\ + \\ f(3)(f(3) - f(1)) + f(3)(f(3) - f(2)) + f(3)(f(3) - f(4)) \\ + \\ f(4)(f(4) - f(3)) \end{gathered}$$

- **f is a vector and a function?**

Graph Laplacian

$$f(1)(f(1)-f(2)) + f(1)(f(1)-f(3))$$
$$+$$
$$f(2)(f(2)-f(1)) + f(2)(f(2)-f(3))$$
$$+$$
$$f(3)(f(3)-f(1)) + f(3)(f(3)-f(2)) + f(3)(f(3)-f(4))$$
$$+$$
$$f(4)(f(4)-f(3))$$

$$(f(1)-f(2))^2$$
$$+$$
$$(f(1)-f(3))^2$$
$$+$$
$$(f(2)-f(3))^2$$
$$+$$
$$(f(3)-f(4))^2$$

$$\lambda = \sum_i (f(i) \sum_{j, i \sim j} (f(i) - f(j))) = \sum_{i<j, i \sim j} (f(i) - f(j))^2$$

Graph Laplacian

$$\lambda = \sum_{i<j, i\sim j} \boxed{(f(i) - f(j))^2}$$

Observation 1: L is positive semi-definite.

$$\lambda_i > 0 \quad \forall i$$

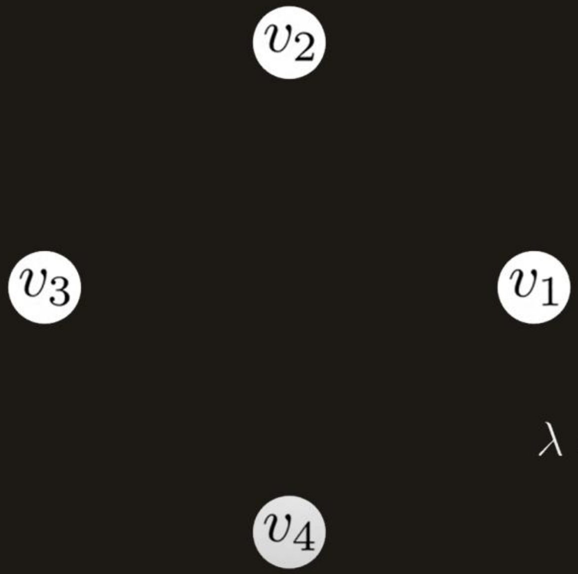
Observation 2: 0 is always an eigenvalue of L.

$$f(i) = f(j) \quad \forall i, j$$

Observation 3a: The smaller the eigenvalue, the *smoother* the eigenvector.

Observation 3b: The smaller the eigenvalue, the less *connected* the graph.

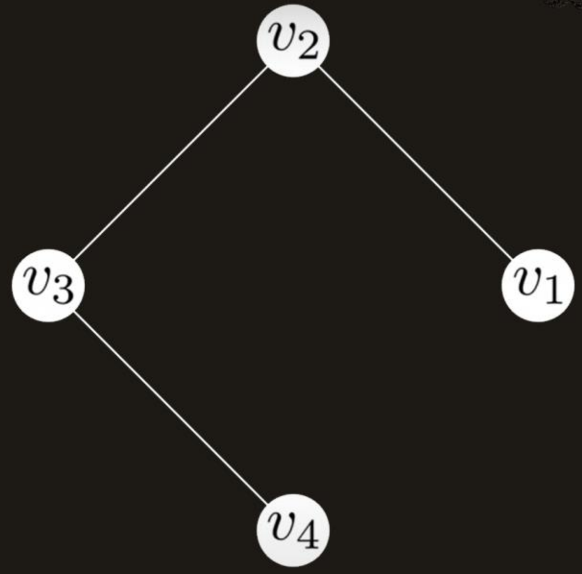
Example: Disconnected Graph



$$L = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

$$\lambda = 0 \quad f_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} f_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} f_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} f_4 = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}$$

Example: Vertices in a Row

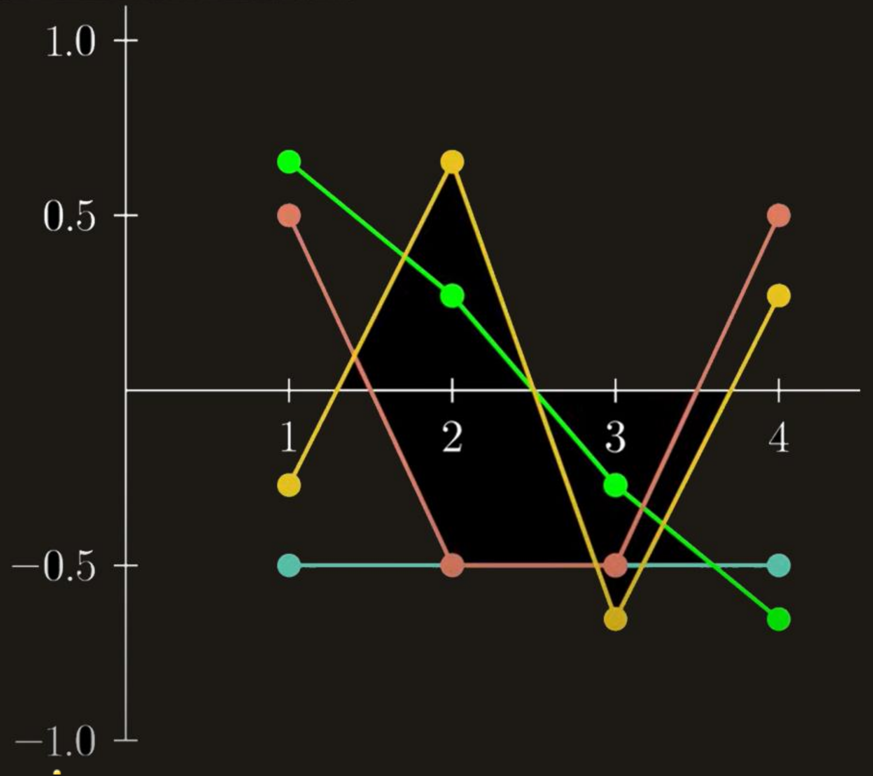


$\lambda_1 = 0 \quad \lambda_2 = 0.59$

$\lambda_3 = 2.0 \quad \lambda_4 = 3.41$

[redacted]

[redacted]



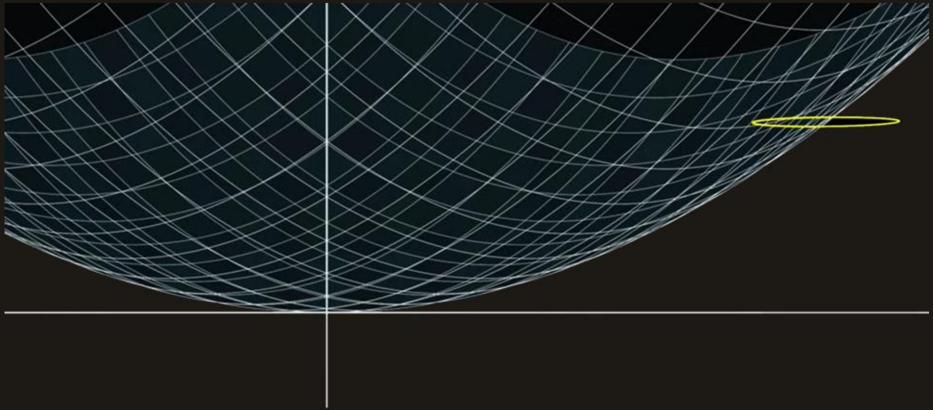
Laplacian Operator

$$\nabla^2 f = \nabla \cdot \nabla f$$

$$\nabla^2 f(x) = \frac{d^2 f}{dx^2}$$

$$\nabla^2 f(x, y) = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2}$$

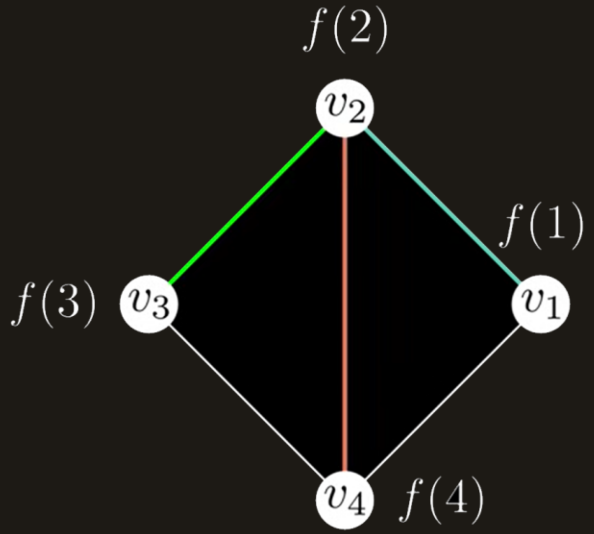
$$\nabla^2 f(x, y, z) = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} + \frac{\partial^2 f}{\partial z^2}$$



$$\nabla^2 f(x, y) \geq 0$$

- **Laplacian operator calculates the divergence of a gradient in Cartesian coordinates**

Why is it called the Laplacian matrix?



$$L = \begin{pmatrix} 2 & -1 & 0 & -1 \\ -1 & 3 & -1 & -1 \\ 0 & -1 & 2 & -1 \\ -1 & -1 & -1 & 3 \end{pmatrix}$$

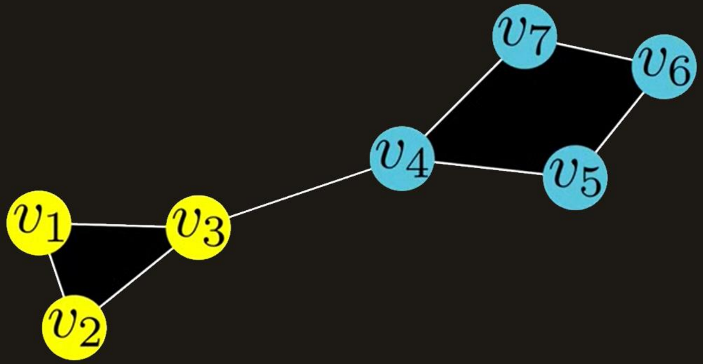
$$(Lf)_i = \sum_{j, i \sim j} (f(i) - f(j))$$

$$(Lf)_2 = (f(2) - f(1)) + (f(2) - f(3)) + (f(2) - f(4))$$

An Application of Laplacian Matrix

Theorem 1: the Laplacian matrix L has an eigenvalue 0 with multiplicity k if and only if the graph has k connected components.

Fiedler Value and Vector of a Graph



$$L = \begin{pmatrix} 2 & -1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 & 0 & 0 \\ -1 & -1 & 3 & \boxed{-1} & 0 & 0 & 0 \\ 0 & 0 & \boxed{-1} & 3 & -1 & 0 & -1 \\ 0 & 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 0 & -1 & 2 \end{pmatrix}$$

$$f_2^T = \begin{pmatrix} 0.48 & 0.48 & 0.31 & -0.15 & -0.35 & -0.42 & -0.35 \end{pmatrix}$$

$$\lambda_2 = 0.36$$

Applications of Laplacian Matrix

$$\lambda_k = \sum_{i<j, i\sim j} w_{ij}(f_k(i) - f_k(j))^2$$

$$f_2 = \underset{f}{\text{argmin}}\ f^T L f, \text{ subject to } f^T 1 = 0, f^T f = 1$$

$$f_3 = \underset{f}{\text{argmin}}\ f^T L f, \text{ subject to } f^T 1 = 0, f^T f_2 = 0, f^T f = 1$$

$$f_k = \underset{f}{\text{argmin}}\ f^T L f, \text{ subject to } f^T 1 = 0, f^T f_2 = 0, \cdots, f^T f_{k-1} = 0, f^T f = 1$$

- **More generally looking for patterns in graph structure can be framed as an optimization problem with weights assigned to graph edges (weighted graph)**

Spectral Embedding

Principal Component Analysis

Dimension reduction

Only on *covariance* matrix

Spectral Embedding

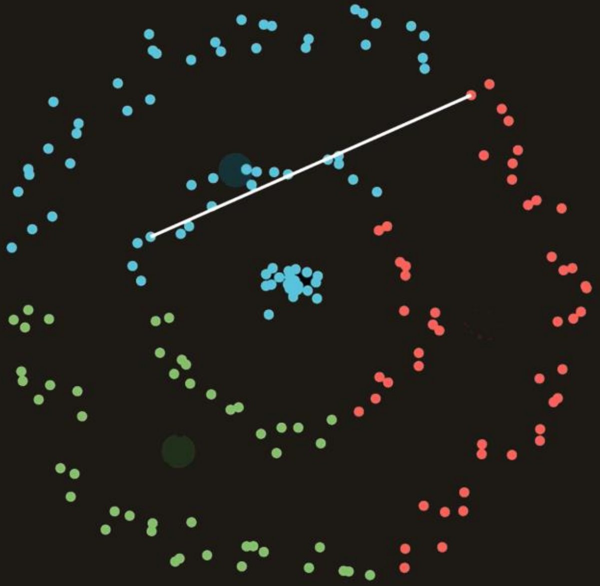
Graph partitioning

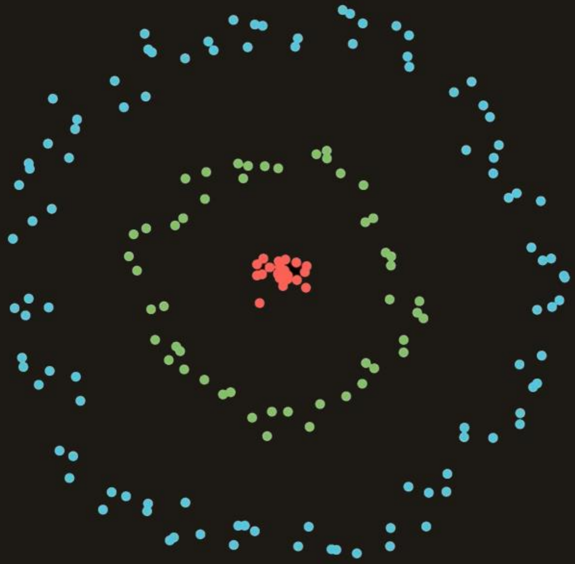
Works on any *similarity* matrix

On spectral clustering: Analysis and an algorithm 12420 2001
A Ng, M Jordan, Y Weiss
Advances in neural information processing systems 14

Spectral Clustering

$$A_{12} = \underbrace{\exp\left(-\frac{\|p_1 - p_2\|^2}{2\sigma^2}\right)}_{\textit{affinity} \text{ between } p_1 \text{ and } p_2}$$





An Invitation to Spectral Graph Theory: Summary

- Graphs can be represented by matrices
- Graph eigenvectors and eigenvalues offer insight into its structure
- Graph Laplacian is a way to perform more complex graph analytics
- Spectral clustering is an application of Spectral Graph Theory in Machine Learning

Special thanks to ***Maxim Beketov*** for guidance, lessons and careful review of slides

THANKS!

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